Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:18 AM GMT

PDB ID	:	3AAT
Title	:	ACTIVITY AND STRUCTURE OF THE ACTIVE-SITE MUTANTS R386Y AND R386F OF ESCHERICHIA COLI ASPARTATE AMINOTRANSFERASE
Authors	:	Danishefsky, A.T.; Ringe, D.; Petsko, G.A.
Deposited on	:	1990-12-06
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

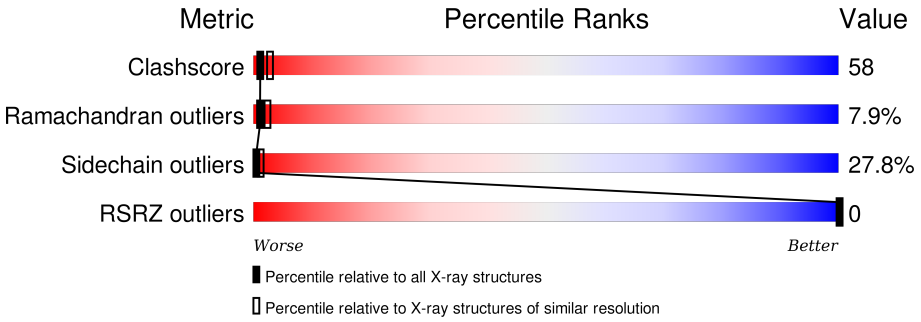
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	396	19% 36% 31% 14%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	411	-	X	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3088 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

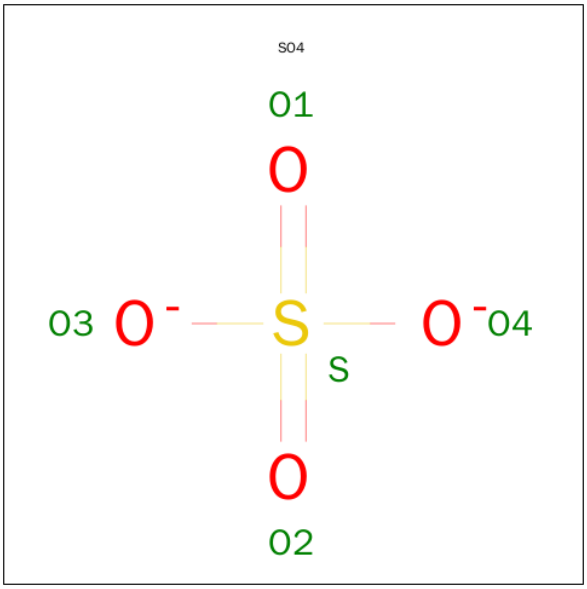
- Molecule 1 is a protein called ASPARTATE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	396	3068	1939	533	583	13	0	0	0

There is a discrepancy between the modelled and reference sequences:

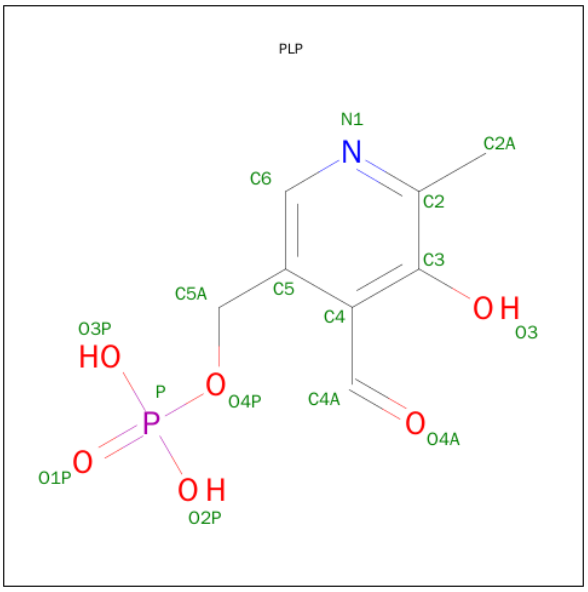
Chain	Residue	Modelled	Actual	Comment	Reference
A	386	PHE	ARG	ENGINEERED MUTATION	UNP P00509

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



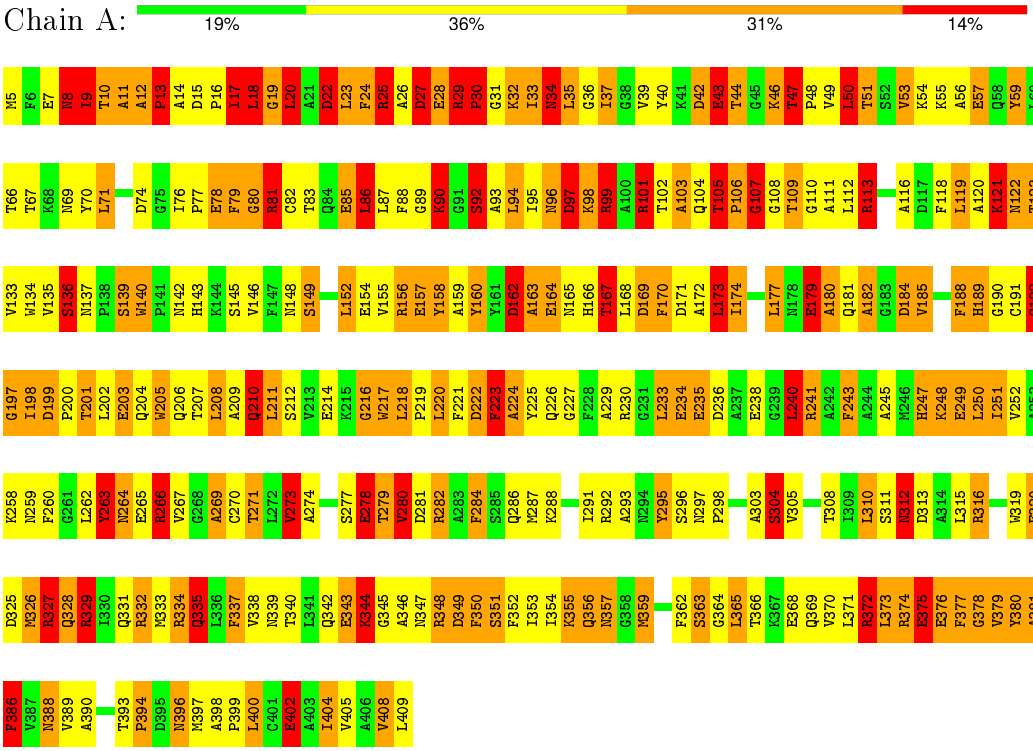
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	15	8	1	5	1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: ASPARTATE AMINOTRANSFERASE

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	156.00Å 87.60Å 78.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.80 38.19 – 2.49	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.80) 54.3 (38.19-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.78 (at 2.48Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.215 , (Not available) 0.203 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	24.0	Xtriage
Anisotropy	0.648	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 79.7	EDS
Estimated twinning fraction	0.022 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.029 for -1/2*h+3/2*k,1/2*h+1/2*k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 10531 reflections (0.009%)	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	3088	wwPDB-VP
Average B, all atoms (Å^2)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, PLP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.04	26/3130 (0.8%)	3.04	365/4242 (8.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	238	GLU	CD-OE2	8.20	1.34	1.25
1	A	376	GLU	CD-OE2	7.84	1.34	1.25
1	A	235	GLU	CD-OE2	7.80	1.34	1.25
1	A	343	GLU	CD-OE2	7.79	1.34	1.25
1	A	7	GLU	CD-OE2	7.78	1.34	1.25
1	A	278	GLU	CD-OE2	7.70	1.34	1.25
1	A	78	GLU	CD-OE2	7.51	1.33	1.25
1	A	320	GLU	CD-OE2	7.27	1.33	1.25
1	A	234	GLU	CD-OE2	7.25	1.33	1.25
1	A	28	GLU	CD-OE2	7.22	1.33	1.25
1	A	386	PHE	CB-CG	-7.19	1.39	1.51
1	A	154	GLU	CD-OE2	7.05	1.33	1.25
1	A	179	GLU	CD-OE2	6.91	1.33	1.25
1	A	402	GLU	CD-OE2	6.74	1.33	1.25
1	A	214	GLU	CD-OE2	6.71	1.33	1.25
1	A	375	GLU	CD-OE2	6.58	1.32	1.25
1	A	43	GLU	CD-OE2	6.54	1.32	1.25
1	A	368	GLU	CD-OE2	6.31	1.32	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	164	GLU	CD-OE2	6.19	1.32	1.25
1	A	203	GLU	CD-OE2	6.03	1.32	1.25
1	A	322	GLU	CD-OE2	5.96	1.32	1.25
1	A	157	GLU	CD-OE2	5.82	1.32	1.25
1	A	386	PHE	CA-CB	-5.77	1.41	1.53
1	A	85	GLU	CD-OE2	5.73	1.31	1.25
1	A	249	GLU	CD-OE2	5.47	1.31	1.25
1	A	62	GLU	CD-OE2	5.40	1.31	1.25

All (365) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	127	ARG	NE-CZ-NH2	23.71	132.16	120.30
1	A	292	ARG	NE-CZ-NH1	22.55	131.58	120.30
1	A	127	ARG	CD-NE-CZ	22.03	154.44	123.60
1	A	334	ARG	NE-CZ-NH1	20.71	130.65	120.30
1	A	59	TYR	CB-CG-CD2	-19.95	109.03	121.00
1	A	327	ARG	NE-CZ-NH2	19.22	129.91	120.30
1	A	59	TYR	CB-CG-CD1	16.69	131.01	121.00
1	A	282	ARG	NE-CZ-NH1	16.10	128.35	120.30
1	A	113	ARG	NE-CZ-NH1	-15.07	112.76	120.30
1	A	349	ASP	CB-CG-OD2	-14.12	105.59	118.30
1	A	313	ASP	CB-CG-OD1	-14.06	105.64	118.30
1	A	81	ARG	NE-CZ-NH1	-14.01	113.29	120.30
1	A	266	ARG	NE-CZ-NH2	-13.76	113.42	120.30
1	A	43	GLU	OE1-CD-OE2	-13.54	107.05	123.30
1	A	113	ARG	NE-CZ-NH2	13.31	126.95	120.30
1	A	365	LEU	CA-CB-CG	12.63	144.34	115.30
1	A	10	THR	C-N-CA	12.62	153.25	121.70
1	A	29	ARG	NE-CZ-NH1	12.38	126.49	120.30
1	A	13	PRO	CB-CA-C	12.32	142.81	112.00
1	A	316	ARG	NE-CZ-NH1	-12.21	114.20	120.30
1	A	334	ARG	NE-CZ-NH2	-12.06	114.27	120.30
1	A	12	ALA	N-CA-C	11.97	143.33	111.00
1	A	241	ARG	NE-CZ-NH1	-11.79	114.41	120.30
1	A	122	ASN	N-CA-CB	11.55	131.39	110.60
1	A	101	ARG	NE-CZ-NH2	11.33	125.97	120.30
1	A	70	TYR	CB-CG-CD2	11.32	127.79	121.00
1	A	105	THR	N-CA-CB	-11.14	89.14	110.30
1	A	43	GLU	CB-CG-CD	10.83	143.43	114.20
1	A	196	THR	OG1-CB-CG2	10.70	134.61	110.00
1	A	230	ARG	NE-CZ-NH1	10.62	125.61	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	127	ARG	NH1-CZ-NH2	-10.61	107.73	119.40
1	A	42	ASP	CB-CG-OD1	10.29	127.56	118.30
1	A	74	ASP	CB-CG-OD1	-10.25	109.08	118.30
1	A	265	GLU	OE1-CD-OE2	-10.15	111.11	123.30
1	A	377	PHE	N-CA-CB	10.08	128.75	110.60
1	A	113	ARG	CD-NE-CZ	10.02	137.62	123.60
1	A	266	ARG	NE-CZ-NH1	9.95	125.28	120.30
1	A	122	ASN	CB-CG-ND2	9.89	140.43	116.70
1	A	146	VAL	CA-CB-CG1	9.86	125.69	110.90
1	A	106	PRO	C-N-CA	9.84	142.96	122.30
1	A	192	CYS	CB-CA-C	9.74	129.88	110.40
1	A	127	ARG	CA-CB-CG	9.72	134.78	113.40
1	A	158	TYR	CB-CG-CD2	9.71	126.83	121.00
1	A	230	ARG	NE-CZ-NH2	9.62	125.11	120.30
1	A	146	VAL	CB-CA-C	9.43	129.32	111.40
1	A	263	TYR	CB-CG-CD2	9.32	126.59	121.00
1	A	230	ARG	NH1-CZ-NH2	-9.24	109.24	119.40
1	A	22	ASP	CB-CG-OD2	-9.18	110.04	118.30
1	A	146	VAL	CA-CB-CG2	-9.13	97.20	110.90
1	A	375	GLU	OE1-CD-OE2	9.02	134.13	123.30
1	A	192	CYS	CA-C-O	9.01	139.01	120.10
1	A	57	GLU	CA-CB-CG	8.99	133.18	113.40
1	A	96	ASN	CB-CA-C	8.90	128.20	110.40
1	A	125	VAL	O-C-N	8.87	136.90	122.70
1	A	34	ASN	N-CA-C	-8.86	87.09	111.00
1	A	35	LEU	N-CA-C	-8.85	87.11	111.00
1	A	12	ALA	N-CA-CB	-8.79	97.80	110.10
1	A	368	GLU	CG-CD-OE1	8.78	135.87	118.30
1	A	11	ALA	N-CA-CB	8.68	122.26	110.10
1	A	349	ASP	CB-CA-C	8.67	127.74	110.40
1	A	157	GLU	OE1-CD-OE2	-8.64	112.94	123.30
1	A	14	ALA	N-CA-C	8.59	134.18	111.00
1	A	89	GLY	CA-C-O	8.59	136.06	120.60
1	A	29	ARG	NH1-CZ-NH2	-8.55	110.00	119.40
1	A	313	ASP	OD1-CG-OD2	8.50	139.44	123.30
1	A	25	ARG	NE-CZ-NH1	8.44	124.52	120.30
1	A	265	GLU	CG-CD-OE1	8.42	135.15	118.30
1	A	245	ALA	CB-CA-C	-8.41	97.48	110.10
1	A	39	VAL	N-CA-CB	-8.30	93.23	111.50
1	A	327	ARG	NE-CZ-NH1	-8.26	116.17	120.30
1	A	372	ARG	NE-CZ-NH1	-8.23	116.19	120.30
1	A	99	ARG	NE-CZ-NH1	-8.17	116.22	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	29	ARG	CD-NE-CZ	8.16	135.02	123.60
1	A	238	GLU	OE1-CD-OE2	8.15	133.09	123.30
1	A	193	HIS	N-CA-CB	-8.14	95.95	110.60
1	A	363	SER	CA-C-O	-8.11	103.07	120.10
1	A	66	THR	N-CA-CB	-8.06	94.99	110.30
1	A	85	GLU	OE1-CD-OE2	8.02	132.92	123.30
1	A	122	ASN	CA-CB-CG	7.99	130.97	113.40
1	A	282	ARG	NH1-CZ-NH2	-7.99	110.61	119.40
1	A	326	MET	CA-CB-CG	-7.96	99.76	113.30
1	A	192	CYS	C-N-CA	7.96	141.59	121.70
1	A	66	THR	CA-CB-CG2	7.92	123.49	112.40
1	A	96	ASN	N-CA-C	-7.88	89.72	111.00
1	A	292	ARG	N-CA-CB	7.88	124.78	110.60
1	A	56	ALA	N-CA-CB	7.87	121.12	110.10
1	A	192	CYS	CA-CB-SG	-7.87	99.83	114.00
1	A	22	ASP	CA-CB-CG	-7.86	96.11	113.40
1	A	10	THR	CB-CA-C	7.84	132.76	111.60
1	A	162	ASP	CB-CG-OD1	7.83	125.35	118.30
1	A	62	GLU	CA-CB-CG	7.79	130.55	113.40
1	A	229	ALA	CB-CA-C	7.78	121.77	110.10
1	A	158	TYR	CB-CG-CD1	-7.77	116.34	121.00
1	A	12	ALA	CB-CA-C	-7.70	98.54	110.10
1	A	200	PRO	N-CA-C	-7.69	92.11	112.10
1	A	199	ASP	CA-CB-CG	7.68	130.29	113.40
1	A	63	ASN	CB-CA-C	7.58	125.55	110.40
1	A	139	SER	N-CA-CB	7.57	121.86	110.50
1	A	280	VAL	CG1-CB-CG2	-7.56	98.81	110.90
1	A	93	ALA	N-CA-CB	7.53	120.65	110.10
1	A	125	VAL	N-CA-C	-7.52	90.69	111.00
1	A	28	GLU	C-N-CA	7.52	140.49	121.70
1	A	162	ASP	CA-CB-CG	7.50	129.90	113.40
1	A	107	GLY	N-CA-C	7.49	131.81	113.10
1	A	263	TYR	CB-CG-CD1	-7.45	116.53	121.00
1	A	343	GLU	CG-CD-OE2	-7.45	103.41	118.30
1	A	321	GLN	CB-CG-CD	7.43	130.92	111.60
1	A	196	THR	CA-CB-CG2	-7.41	102.03	112.40
1	A	292	ARG	NH1-CZ-NH2	-7.40	111.26	119.40
1	A	365	LEU	CB-CG-CD2	7.36	123.52	111.00
1	A	374	ARG	CG-CD-NE	7.34	127.22	111.80
1	A	321	GLN	CG-CD-OE1	7.30	136.21	121.60
1	A	400	LEU	CA-CB-CG	7.28	132.04	115.30
1	A	234	GLU	CA-C-N	7.27	133.19	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	386	PHE	CA-CB-CG	7.21	131.20	113.90
1	A	127	ARG	CG-CD-NE	7.19	126.90	111.80
1	A	24	PHE	O-C-N	7.18	134.19	122.70
1	A	279	THR	O-C-N	7.17	134.18	122.70
1	A	322	GLU	CA-C-O	7.16	135.15	120.10
1	A	236	ASP	CB-CA-C	7.13	124.67	110.40
1	A	334	ARG	N-CA-CB	7.13	123.43	110.60
1	A	199	ASP	CB-CG-OD1	7.10	124.69	118.30
1	A	18	LEU	CA-CB-CG	7.09	131.61	115.30
1	A	105	THR	CA-CB-CG2	7.07	122.30	112.40
1	A	316	ARG	CA-CB-CG	7.06	128.93	113.40
1	A	8	ASN	C-N-CA	7.03	139.28	121.70
1	A	13	PRO	C-N-CA	7.02	139.25	121.70
1	A	216	GLY	O-C-N	-7.02	111.47	122.70
1	A	356	GLN	CA-CB-CG	-7.00	98.01	113.40
1	A	188	PHE	N-CA-CB	6.99	123.18	110.60
1	A	328	GLN	CA-CB-CG	-6.98	98.04	113.40
1	A	233	LEU	CB-CA-C	6.92	123.35	110.20
1	A	223	PHE	CA-C-O	6.91	134.61	120.10
1	A	154	GLU	N-CA-CB	6.91	123.04	110.60
1	A	189	HIS	O-C-N	6.90	134.93	123.20
1	A	257	SER	N-CA-CB	6.90	120.85	110.50
1	A	235	GLU	CG-CD-OE1	6.87	132.04	118.30
1	A	106	PRO	CA-C-O	6.84	136.61	120.20
1	A	63	ASN	N-CA-CB	-6.83	98.30	110.60
1	A	139	SER	CA-CB-OG	6.83	129.63	111.20
1	A	18	LEU	CB-CA-C	6.80	123.13	110.20
1	A	295	TYR	CB-CG-CD2	6.79	125.07	121.00
1	A	335	GLN	CA-CB-CG	6.79	128.33	113.40
1	A	195	PRO	N-CD-CG	-6.77	93.05	103.20
1	A	70	TYR	CB-CG-CD1	-6.76	116.94	121.00
1	A	195	PRO	CA-C-O	-6.74	104.03	120.20
1	A	214	GLU	OE1-CD-OE2	-6.73	115.23	123.30
1	A	321	GLN	OE1-CD-NE2	-6.73	106.42	121.90
1	A	235	GLU	CG-CD-OE2	-6.72	104.85	118.30
1	A	332	ARG	CD-NE-CZ	6.71	133.00	123.60
1	A	120	ALA	CB-CA-C	6.71	120.16	110.10
1	A	214	GLU	CB-CG-CD	6.70	132.29	114.20
1	A	50	LEU	CB-CG-CD1	-6.70	99.61	111.00
1	A	14	ALA	CA-C-O	6.69	134.15	120.10
1	A	64	GLU	OE1-CD-OE2	6.68	131.31	123.30
1	A	98	LYS	CA-CB-CG	6.68	128.09	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	14	ALA	O-C-N	-6.68	112.02	122.70
1	A	156	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	A	192	CYS	CA-C-N	-6.67	102.51	117.20
1	A	375	GLU	CG-CD-OE2	-6.63	105.04	118.30
1	A	304	SER	O-C-N	6.63	133.30	122.70
1	A	184	ASP	CB-CG-OD2	-6.62	112.35	118.30
1	A	250	LEU	CB-CA-C	6.62	122.77	110.20
1	A	136	SER	N-CA-CB	6.61	120.41	110.50
1	A	11	ALA	CB-CA-C	-6.60	100.20	110.10
1	A	320	GLU	OE1-CD-OE2	-6.56	115.42	123.30
1	A	74	ASP	CB-CA-C	6.52	123.44	110.40
1	A	281	ASP	CB-CG-OD2	-6.52	112.44	118.30
1	A	348	ARG	CA-C-N	-6.52	102.86	117.20
1	A	169	ASP	O-C-N	6.50	133.10	122.70
1	A	234	GLU	O-C-N	-6.47	112.35	122.70
1	A	357	ASN	CA-CB-CG	6.46	127.61	113.40
1	A	189	HIS	CA-C-O	-6.45	106.56	120.10
1	A	368	GLU	CG-CD-OE2	-6.44	105.42	118.30
1	A	22	ASP	CA-C-O	-6.42	106.61	120.10
1	A	356	GLN	N-CA-CB	-6.42	99.05	110.60
1	A	388	ASN	CB-CG-OD1	6.42	134.43	121.60
1	A	210	GLN	CB-CG-CD	6.39	128.23	111.60
1	A	81	ARG	NH1-CZ-NH2	6.39	126.43	119.40
1	A	29	ARG	NE-CZ-NH2	6.39	123.50	120.30
1	A	388	ASN	CB-CG-ND2	-6.39	101.37	116.70
1	A	171	ASP	CA-C-O	-6.37	106.72	120.10
1	A	292	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	A	99	ARG	NH1-CZ-NH2	6.31	126.34	119.40
1	A	292	ARG	CD-NE-CZ	6.30	132.42	123.60
1	A	96	ASN	N-CA-CB	6.26	121.88	110.60
1	A	89	GLY	CA-C-N	-6.25	103.44	117.20
1	A	148	ASN	N-CA-CB	6.25	121.85	110.60
1	A	256	TYR	CG-CD1-CE1	-6.25	116.30	121.30
1	A	43	GLU	N-CA-CB	6.24	121.84	110.60
1	A	402	GLU	CA-CB-CG	6.24	127.13	113.40
1	A	51	THR	CA-CB-OG1	-6.24	95.91	109.00
1	A	221	PHE	N-CA-CB	6.23	121.81	110.60
1	A	349	ASP	OD1-CG-OD2	6.22	135.12	123.30
1	A	222	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	A	123	THR	O-C-N	6.19	132.61	122.70
1	A	195	PRO	CA-C-N	6.16	130.74	117.20
1	A	250	LEU	N-CA-CB	-6.12	98.16	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	190	GLY	CA-C-O	6.11	131.60	120.60
1	A	210	GLN	N-CA-CB	6.11	121.60	110.60
1	A	345	GLY	N-CA-C	6.10	128.35	113.10
1	A	172	ALA	CB-CA-C	-6.08	100.98	110.10
1	A	375	GLU	O-C-N	-6.07	112.98	122.70
1	A	113	ARG	CA-CB-CG	-6.07	100.04	113.40
1	A	169	ASP	CB-CG-OD2	-6.07	112.84	118.30
1	A	255	SER	CB-CA-C	6.06	121.62	110.10
1	A	381	ALA	N-CA-CB	6.04	118.56	110.10
1	A	269	ALA	CB-CA-C	6.03	119.14	110.10
1	A	376	GLU	N-CA-CB	6.02	121.43	110.60
1	A	394	PRO	O-C-N	6.01	132.31	122.70
1	A	28	GLU	CA-CB-CG	5.98	126.56	113.40
1	A	173	LEU	CA-CB-CG	5.97	129.04	115.30
1	A	282	ARG	CB-CG-CD	5.97	127.11	111.60
1	A	316	ARG	N-CA-CB	5.95	121.31	110.60
1	A	156	ARG	CA-CB-CG	5.94	126.47	113.40
1	A	22	ASP	CA-C-N	5.93	130.26	117.20
1	A	222	ASP	O-C-N	5.93	132.18	122.70
1	A	332	ARG	NE-CZ-NH2	5.93	123.26	120.30
1	A	199	ASP	CB-CA-C	-5.92	98.55	110.40
1	A	350	PHE	CA-CB-CG	5.92	128.11	113.90
1	A	264	ASN	CB-CG-OD1	-5.91	109.78	121.60
1	A	273	VAL	CB-CA-C	5.91	122.63	111.40
1	A	279	THR	CA-C-O	-5.91	107.69	120.10
1	A	19	GLY	N-CA-C	-5.90	98.34	113.10
1	A	50	LEU	N-CA-C	5.90	126.92	111.00
1	A	53	VAL	CA-CB-CG1	5.88	119.72	110.90
1	A	385	GLY	O-C-N	5.87	132.10	122.70
1	A	256	TYR	O-C-N	5.86	132.08	122.70
1	A	37	ILE	C-N-CA	-5.84	110.04	122.30
1	A	320	GLU	CG-CD-OE1	5.84	129.98	118.30
1	A	29	ARG	N-CA-C	-5.82	95.29	111.00
1	A	189	HIS	N-CA-C	-5.81	95.31	111.00
1	A	349	ASP	CA-CB-CG	-5.81	100.63	113.40
1	A	222	ASP	N-CA-CB	5.78	121.01	110.60
1	A	81	ARG	CD-NE-CZ	5.77	131.68	123.60
1	A	156	ARG	CD-NE-CZ	5.77	131.68	123.60
1	A	278	GLU	OE1-CD-OE2	5.77	130.22	123.30
1	A	380	TYR	CA-CB-CG	-5.77	102.44	113.40
1	A	162	ASP	CB-CA-C	5.76	121.92	110.40
1	A	8	ASN	CA-C-N	-5.75	104.55	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	34	ASN	O-C-N	5.75	131.90	122.70
1	A	191	CYS	CA-CB-SG	-5.75	103.65	114.00
1	A	99	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	A	34	ASN	N-CA-CB	5.73	120.92	110.60
1	A	83	THR	CA-CB-CG2	-5.71	104.40	112.40
1	A	356	GLN	OE1-CD-NE2	5.71	135.03	121.90
1	A	194	ASN	CA-CB-CG	5.69	125.92	113.40
1	A	408	VAL	C-N-CA	5.69	135.91	121.70
1	A	121	LYS	N-CA-C	-5.68	95.66	111.00
1	A	329	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	A	122	ASN	N-CA-C	-5.67	95.70	111.00
1	A	48	PRO	CA-C-N	-5.65	104.77	117.20
1	A	298	PRO	N-CA-CB	-5.65	96.39	102.60
1	A	94	LEU	O-C-N	5.65	131.74	122.70
1	A	288	LYS	CA-CB-CG	5.65	125.82	113.40
1	A	70	TYR	N-CA-CB	5.63	120.74	110.60
1	A	342	GLN	CA-C-O	5.62	131.91	120.10
1	A	8	ASN	CA-C-O	5.61	131.88	120.10
1	A	303	ALA	N-CA-CB	-5.61	102.24	110.10
1	A	18	LEU	CA-C-N	-5.61	104.99	116.20
1	A	280	VAL	N-CA-CB	5.60	123.82	111.50
1	A	9	ILE	CB-CG1-CD1	5.58	129.53	113.90
1	A	122	ASN	CB-CG-OD1	-5.58	110.44	121.60
1	A	295	TYR	N-CA-C	-5.58	95.95	111.00
1	A	247	HIS	CA-CB-CG	-5.57	104.13	113.60
1	A	230	ARG	C-N-CA	-5.56	110.61	122.30
1	A	190	GLY	O-C-N	-5.56	113.80	122.70
1	A	169	ASP	OD1-CG-OD2	5.56	133.86	123.30
1	A	122	ASN	OD1-CG-ND2	-5.56	109.12	121.90
1	A	169	ASP	CB-CG-OD1	-5.56	113.30	118.30
1	A	17	ILE	O-C-N	5.55	131.58	122.70
1	A	278	GLU	CA-C-O	5.55	131.75	120.10
1	A	5	MET	CA-CB-CG	-5.52	103.91	113.30
1	A	227	GLY	O-C-N	5.52	131.53	122.70
1	A	380	TYR	CB-CG-CD2	5.52	124.31	121.00
1	A	340	THR	CA-CB-CG2	5.51	120.12	112.40
1	A	312	ASN	OD1-CG-ND2	5.51	134.57	121.90
1	A	375	GLU	N-CA-CB	5.50	120.51	110.60
1	A	386	PHE	CD1-CG-CD2	5.50	125.45	118.30
1	A	44	THR	CA-CB-OG1	-5.48	97.49	109.00
1	A	82	CYS	CB-CA-C	5.48	121.35	110.40
1	A	386	PHE	CB-CA-C	5.47	121.34	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	20	LEU	O-C-N	5.46	131.44	122.70
1	A	29	ARG	CA-CB-CG	5.46	125.41	113.40
1	A	22	ASP	OD1-CG-OD2	5.46	133.67	123.30
1	A	174	ILE	CA-C-O	5.46	131.56	120.10
1	A	278	GLU	CB-CG-CD	5.45	128.92	114.20
1	A	322	GLU	O-C-N	-5.45	113.98	122.70
1	A	379	VAL	CB-CA-C	5.44	121.74	111.40
1	A	312	ASN	CA-C-O	-5.44	108.68	120.10
1	A	195	PRO	CA-N-CD	-5.43	103.90	111.50
1	A	50	LEU	CA-CB-CG	-5.43	102.82	115.30
1	A	92	SER	CB-CA-C	-5.42	99.80	110.10
1	A	126	LYS	CA-C-O	-5.42	108.72	120.10
1	A	257	SER	CA-CB-OG	5.42	125.84	111.20
1	A	278	GLU	CG-CD-OE1	-5.42	107.47	118.30
1	A	110	GLY	CA-C-O	5.41	130.34	120.60
1	A	247	HIS	CA-C-O	-5.41	108.75	120.10
1	A	27	ASP	O-C-N	5.39	131.32	122.70
1	A	343	GLU	N-CA-CB	-5.38	100.91	110.60
1	A	359	MET	CG-SD-CE	5.37	108.78	100.20
1	A	402	GLU	CA-C-O	5.35	131.34	120.10
1	A	224	ALA	CA-C-O	-5.35	108.87	120.10
1	A	137	ASN	N-CA-CB	5.35	120.22	110.60
1	A	240	LEU	CA-CB-CG	5.34	127.59	115.30
1	A	57	GLU	CG-CD-OE2	5.34	128.99	118.30
1	A	70	TYR	CA-CB-CG	5.34	123.55	113.40
1	A	281	ASP	CB-CG-OD1	5.33	123.09	118.30
1	A	308	THR	CA-CB-OG1	-5.32	97.82	109.00
1	A	64	GLU	CG-CD-OE2	-5.32	107.67	118.30
1	A	383	ALA	CA-C-O	-5.32	108.94	120.10
1	A	310	LEU	CB-CA-C	5.31	120.29	110.20
1	A	386	PHE	CB-CG-CD1	-5.31	117.08	120.80
1	A	106	PRO	O-C-N	-5.30	114.19	123.20
1	A	90	LYS	CB-CA-C	5.30	121.00	110.40
1	A	296	SER	CA-CB-OG	5.30	125.50	111.20
1	A	250	LEU	CB-CG-CD1	-5.30	102.00	111.00
1	A	394	PRO	CA-C-O	-5.29	107.50	120.20
1	A	59	TYR	OH-CZ-CE2	-5.29	105.83	120.10
1	A	199	ASP	OD1-CG-OD2	-5.28	113.27	123.30
1	A	235	GLU	CA-C-O	5.28	131.19	120.10
1	A	122	ASN	O-C-N	5.27	131.13	122.70
1	A	296	SER	CA-C-N	5.27	128.79	117.20
1	A	363	SER	N-CA-C	-5.26	96.79	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	377	PHE	O-C-N	5.26	132.15	123.20
1	A	157	GLU	CG-CD-OE1	5.26	128.82	118.30
1	A	208	LEU	CB-CA-C	5.26	120.19	110.20
1	A	7	GLU	CB-CG-CD	5.25	128.39	114.20
1	A	86	LEU	CB-CA-C	5.25	120.18	110.20
1	A	251	ILE	CB-CG1-CD1	-5.25	99.21	113.90
1	A	223	PHE	N-CA-CB	-5.24	101.16	110.60
1	A	146	VAL	CG1-CB-CG2	-5.24	102.51	110.90
1	A	113	ARG	N-CA-CB	5.24	120.03	110.60
1	A	157	GLU	CB-CG-CD	5.24	128.34	114.20
1	A	167	THR	O-C-N	5.22	131.06	122.70
1	A	311	SER	CA-CB-OG	-5.22	97.11	111.20
1	A	207	THR	CA-CB-CG2	5.20	119.68	112.40
1	A	292	ARG	CA-CB-CG	5.20	124.83	113.40
1	A	28	GLU	N-CA-C	5.19	125.02	111.00
1	A	170	PHE	CB-CA-C	-5.19	100.02	110.40
1	A	126	LYS	O-C-N	5.19	131.00	122.70
1	A	140	TRP	CB-CA-C	5.19	120.78	110.40
1	A	344	LYS	CG-CD-CE	5.18	127.43	111.90
1	A	30	PRO	C-N-CA	5.17	133.16	122.30
1	A	223	PHE	C-N-CA	5.16	134.61	121.70
1	A	18	LEU	CA-C-O	5.16	130.93	120.10
1	A	340	THR	CB-CA-C	5.15	125.51	111.60
1	A	374	ARG	CA-C-O	-5.15	109.28	120.10
1	A	79	PHE	N-CA-CB	-5.15	101.33	110.60
1	A	378	GLY	CA-C-O	-5.14	111.34	120.60
1	A	348	ARG	CA-C-O	5.13	130.88	120.10
1	A	191	CYS	C-N-CA	5.13	134.53	121.70
1	A	43	GLU	CG-CD-OE1	5.11	128.52	118.30
1	A	214	GLU	O-C-N	5.11	130.87	122.70
1	A	25	ARG	CD-NE-CZ	5.09	130.73	123.60
1	A	284	PHE	CB-CA-C	5.09	120.58	110.40
1	A	22	ASP	N-CA-CB	5.07	119.72	110.60
1	A	64	GLU	C-N-CA	5.07	134.37	121.70
1	A	103	ALA	CA-C-O	5.07	130.74	120.10
1	A	337	PHE	CA-C-O	5.07	130.74	120.10
1	A	365	LEU	CB-CG-CD1	-5.06	102.39	111.00
1	A	47	THR	N-CA-CB	-5.06	100.69	110.30
1	A	13	PRO	CA-N-CD	-5.04	104.45	111.50
1	A	342	GLN	CA-C-N	-5.01	106.17	117.20
1	A	28	GLU	CG-CD-OE1	5.00	128.31	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	25	ARG	Sidechain
1	A	327	ARG	Sidechain
1	A	81	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3068	0	3010	351	0
2	A	5	0	0	0	0
3	A	15	0	6	3	0
All	All	3088	0	3016	351	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 58.

All (351) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:LYS:HB3	1:A:248:LYS:NZ	1.52	1.18
1:A:247:HIS:O	1:A:248:LYS:HB2	1.56	1.04
1:A:96:ASN:O	1:A:97:ASP:HB2	1.57	1.01
1:A:32:LYS:HE2	1:A:400:LEU:HD13	1.42	0.99
1:A:34:ASN:HB2	1:A:36:GLY:H	1.26	0.99
1:A:20:LEU:HD13	1:A:382:VAL:HG23	1.47	0.96
1:A:92:SER:HB3	1:A:95:ILE:HD12	1.47	0.95
1:A:337:PHE:HD1	1:A:397:MET:HE1	1.29	0.95
1:A:125:VAL:HG11	1:A:185:VAL:HG12	1.48	0.94
1:A:195:PRO:HB2	1:A:362:PHE:HE1	1.31	0.94
1:A:34:ASN:HA	1:A:380:TYR:HB2	1.50	0.93
1:A:123:THR:HG22	1:A:125:VAL:HG22	1.51	0.93
1:A:50:LEU:N	1:A:50:LEU:HD12	1.84	0.92
1:A:27:ASP:HB3	1:A:380:TYR:OH	1.71	0.90
1:A:248:LYS:HZ2	1:A:248:LYS:HB3	1.09	0.89
1:A:375:GLU:CD	1:A:376:GLU:H	1.75	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ALA:HA	1:A:216:GLY:HA3	1.56	0.87
1:A:32:LYS:HB2	1:A:379:VAL:HG12	1.57	0.85
1:A:20:LEU:HD11	1:A:382:VAL:HA	1.57	0.85
1:A:29:ARG:HH11	1:A:378:GLY:HA2	1.41	0.85
1:A:19:GLY:O	1:A:20:LEU:HB2	1.76	0.84
1:A:24:PHE:CZ	1:A:33:ILE:HA	2.11	0.84
1:A:346:ALA:HB2	1:A:405:VAL:HG12	1.61	0.82
1:A:347:ASN:HD21	1:A:409:LEU:HD13	1.43	0.82
1:A:160:TYR:O	1:A:168:LEU:HD12	1.79	0.81
1:A:123:THR:CG2	1:A:125:VAL:HG22	2.10	0.81
1:A:256:TYR:HB2	1:A:267:VAL:HG23	1.59	0.81
1:A:250:LEU:HD12	1:A:251:ILE:H	1.43	0.81
1:A:375:GLU:OE1	1:A:376:GLU:N	2.15	0.80
1:A:256:TYR:HB2	1:A:267:VAL:CG2	2.11	0.79
1:A:29:ARG:HB3	1:A:30:PRO:CD	2.13	0.79
1:A:220:LEU:HA	1:A:251:ILE:HG23	1.63	0.79
1:A:180:ALA:O	1:A:181:GLN:HB3	1.83	0.78
1:A:20:LEU:CD1	1:A:382:VAL:HA	2.15	0.77
1:A:18:LEU:CD1	1:A:22:ASP:HB2	2.15	0.77
1:A:195:PRO:HB2	1:A:362:PHE:CE1	2.18	0.77
1:A:34:ASN:HB2	1:A:36:GLY:N	2.00	0.76
1:A:328:GLN:HG3	1:A:331:GLN:NE2	2.01	0.76
1:A:260:PHE:CZ	1:A:310:LEU:HD21	2.21	0.75
1:A:205:TRP:CE3	1:A:205:TRP:HA	2.20	0.75
1:A:18:LEU:HD13	1:A:22:ASP:HB2	1.69	0.75
1:A:388:ASN:OD1	1:A:390:ALA:HB3	1.87	0.75
1:A:355:LYS:NZ	1:A:355:LYS:HB2	2.01	0.75
1:A:355:LYS:HZ3	1:A:355:LYS:HB2	1.52	0.75
1:A:375:GLU:CD	1:A:376:GLU:N	2.40	0.75
1:A:26:ALA:O	1:A:28:GLU:HG2	1.87	0.74
1:A:44:THR:HB	1:A:46:LYS:NZ	2.01	0.74
1:A:102:THR:OG1	1:A:271:THR:HG23	1.87	0.74
1:A:256:TYR:O	1:A:260:PHE:HB2	1.87	0.74
1:A:33:ILE:HG22	1:A:34:ASN:H	1.52	0.73
1:A:248:LYS:HZ3	1:A:248:LYS:HB3	1.54	0.73
1:A:76:ILE:HG12	1:A:104:GLN:HE22	1.52	0.73
1:A:23:LEU:O	1:A:27:ASP:HB2	1.87	0.72
1:A:248:LYS:NZ	1:A:249:GLU:HG3	2.04	0.72
1:A:32:LYS:HE2	1:A:400:LEU:CD1	2.19	0.72
1:A:250:LEU:HD12	1:A:251:ILE:N	2.03	0.72
1:A:366:THR:HG22	1:A:369:GLN:HG3	1.72	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:LYS:NZ	1:A:46:LYS:HB2	2.05	0.72
1:A:32:LYS:HE2	1:A:400:LEU:HB2	1.70	0.71
1:A:32:LYS:CE	1:A:400:LEU:HD13	2.18	0.71
1:A:44:THR:HB	1:A:46:LYS:HZ2	1.56	0.71
1:A:12:ALA:O	1:A:13:PRO:C	2.28	0.71
1:A:192:CYS:SG	1:A:199:ASP:HA	2.30	0.71
1:A:23:LEU:HD12	1:A:23:LEU:H	1.54	0.70
1:A:223:PHE:HE1	1:A:240:LEU:HB2	1.54	0.70
1:A:248:LYS:CB	1:A:248:LYS:NZ	2.41	0.70
1:A:127:ARG:NH2	1:A:179:GLU:OE2	2.24	0.70
1:A:374:ARG:HG2	1:A:379:VAL:O	1.91	0.70
1:A:173:LEU:HD12	1:A:177:LEU:HD22	1.73	0.70
1:A:43:GLU:OE2	1:A:329:ARG:HD2	1.91	0.69
1:A:27:ASP:CB	1:A:380:TYR:OH	2.40	0.69
1:A:9:ILE:O	1:A:10:THR:OG1	2.10	0.69
1:A:352:PHE:HD2	1:A:356:GLN:HE22	1.39	0.69
1:A:17:ILE:HG23	1:A:18:LEU:H	1.55	0.69
1:A:337:PHE:CD1	1:A:397:MET:HE1	2.20	0.69
1:A:105:THR:HG22	1:A:107:GLY:HA2	1.75	0.69
1:A:34:ASN:HA	1:A:380:TYR:CB	2.23	0.68
1:A:32:LYS:CB	1:A:379:VAL:HG12	2.23	0.68
1:A:247:HIS:O	1:A:248:LYS:CB	2.35	0.68
1:A:121:LYS:HD2	1:A:122:ASN:N	2.09	0.68
1:A:209:ALA:HB2	1:A:243:PHE:CD1	2.29	0.67
1:A:196:THR:HB	1:A:198:ILE:HD11	1.76	0.67
1:A:160:TYR:HE1	1:A:198:ILE:HD13	1.60	0.67
1:A:173:LEU:CD1	1:A:177:LEU:HD22	2.25	0.67
1:A:109:THR:HG22	1:A:140:TRP:CH2	2.30	0.67
1:A:260:PHE:HZ	1:A:310:LEU:HD21	1.59	0.67
1:A:233:LEU:HD21	1:A:319:TRP:CH2	2.29	0.67
1:A:29:ARG:HB3	1:A:30:PRO:HD3	1.75	0.67
1:A:362:PHE:CD1	1:A:386:PHE:HB3	2.31	0.66
1:A:9:ILE:HD13	1:A:10:THR:N	2.09	0.66
1:A:105:THR:HG21	1:A:111:ALA:HB2	1.76	0.66
1:A:29:ARG:CB	1:A:30:PRO:CD	2.74	0.66
1:A:125:VAL:CG1	1:A:185:VAL:HG12	2.26	0.66
1:A:87:LEU:HB3	1:A:240:LEU:HD11	1.76	0.66
1:A:352:PHE:HD2	1:A:356:GLN:NE2	1.94	0.65
1:A:87:LEU:O	1:A:241:ARG:HD2	1.96	0.65
1:A:224:ALA:O	1:A:225:TYR:HB2	1.96	0.65
1:A:62:GLU:HG3	1:A:63:ASN:ND2	2.11	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:ARG:NH1	1:A:149:SER:OG	2.30	0.64
1:A:366:THR:HG22	1:A:369:GLN:CG	2.28	0.64
1:A:121:LYS:C	1:A:121:LYS:HD2	2.18	0.63
1:A:251:ILE:O	1:A:251:ILE:HG23	1.97	0.63
1:A:126:LYS:HD3	1:A:126:LYS:N	2.13	0.63
1:A:135:VAL:O	1:A:136:SER:HB3	1.97	0.63
1:A:87:LEU:HB3	1:A:240:LEU:CD1	2.28	0.63
1:A:197:GLY:HA3	1:A:357:ASN:O	1.98	0.63
1:A:81:ARG:O	1:A:85:GLU:HG3	1.98	0.63
1:A:159:ALA:O	1:A:160:TYR:HB2	1.99	0.62
1:A:160:TYR:HE1	1:A:198:ILE:CD1	2.11	0.62
1:A:20:LEU:CD1	1:A:382:VAL:HG23	2.26	0.62
1:A:20:LEU:HD21	1:A:381:ALA:C	2.19	0.62
1:A:362:PHE:HA	1:A:386:PHE:HA	1.80	0.62
1:A:50:LEU:H	1:A:50:LEU:HD12	1.64	0.62
1:A:400:LEU:O	1:A:404:ILE:HD13	2.01	0.61
1:A:203:GLU:O	1:A:206:GLN:HB2	2.00	0.61
1:A:46:LYS:HB2	1:A:46:LYS:HZ3	1.66	0.60
1:A:181:GLN:O	1:A:184:ASP:HB2	2.01	0.60
1:A:121:LYS:C	1:A:123:THR:H	2.04	0.60
1:A:404:ILE:O	1:A:408:VAL:HG22	2.02	0.60
1:A:23:LEU:HD12	1:A:23:LEU:N	2.17	0.60
1:A:43:GLU:HG3	1:A:394:PRO:HD3	1.83	0.59
1:A:105:THR:O	1:A:107:GLY:N	2.35	0.59
1:A:62:GLU:HG3	1:A:63:ASN:HD22	1.66	0.59
1:A:375:GLU:C	1:A:377:PHE:H	2.05	0.59
1:A:90:LYS:HA	1:A:90:LYS:NZ	2.18	0.59
1:A:349:ASP:OD1	1:A:351:SER:HB3	2.03	0.58
1:A:398:ALA:HB3	1:A:399:PRO:CD	2.33	0.58
1:A:92:SER:CB	1:A:95:ILE:HD12	2.27	0.58
1:A:76:ILE:CG1	1:A:104:GLN:HE22	2.16	0.58
1:A:43:GLU:HG3	1:A:394:PRO:CD	2.33	0.58
1:A:43:GLU:CD	1:A:329:ARG:HD2	2.24	0.58
1:A:408:VAL:O	1:A:409:LEU:HG	2.03	0.58
1:A:160:TYR:CE1	1:A:198:ILE:HD13	2.38	0.58
1:A:248:LYS:HZ1	1:A:249:GLU:HG3	1.68	0.58
1:A:328:GLN:HA	1:A:331:GLN:HE21	1.68	0.57
1:A:350:PHE:HA	1:A:352:PHE:CD1	2.40	0.57
1:A:77:PRO:HG2	1:A:78:GLU:OE1	2.05	0.57
1:A:328:GLN:O	1:A:332:ARG:HG3	2.03	0.57
1:A:163:ALA:O	1:A:165:ASN:N	2.38	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ALA:O	1:A:269:ALA:HB1	2.05	0.57
1:A:96:ASN:O	1:A:97:ASP:CB	2.41	0.56
1:A:312:ASN:HD22	1:A:312:ASN:C	2.07	0.56
1:A:29:ARG:NH1	1:A:378:GLY:HA2	2.18	0.56
1:A:34:ASN:CB	1:A:36:GLY:H	2.07	0.56
1:A:196:THR:O	1:A:198:ILE:N	2.36	0.56
1:A:225:TYR:CE2	1:A:258:LYS:HG3	2.39	0.56
1:A:118:PHE:O	1:A:121:LYS:O	2.23	0.56
1:A:34:ASN:N	1:A:34:ASN:OD1	2.38	0.56
1:A:76:ILE:HB	1:A:79:PHE:HB3	1.89	0.55
1:A:50:LEU:N	1:A:50:LEU:CD1	2.63	0.55
1:A:359:MET:O	1:A:389:VAL:N	2.37	0.55
1:A:17:ILE:HG12	1:A:18:LEU:N	2.21	0.55
1:A:196:THR:HB	1:A:198:ILE:CD1	2.36	0.55
1:A:34:ASN:C	1:A:36:GLY:H	2.02	0.55
1:A:17:ILE:C	1:A:19:GLY:N	2.60	0.55
1:A:346:ALA:HB2	1:A:405:VAL:CG1	2.35	0.55
1:A:119:LEU:O	1:A:123:THR:HB	2.08	0.54
1:A:192:CYS:SG	1:A:199:ASP:CA	2.95	0.54
1:A:18:LEU:HD12	1:A:22:ASP:HB2	1.87	0.54
1:A:355:LYS:CB	1:A:355:LYS:NZ	2.70	0.54
1:A:40:TYR:O	1:A:47:THR:HB	2.06	0.54
1:A:101:ARG:HB3	1:A:284:PHE:CD1	2.43	0.54
1:A:160:TYR:O	1:A:168:LEU:CD1	2.55	0.54
1:A:201:THR:OG1	1:A:204:GLN:NE2	2.39	0.54
1:A:397:MET:HE3	1:A:400:LEU:HD21	1.88	0.54
1:A:121:LYS:NZ	1:A:122:ASN:HB2	2.22	0.53
1:A:328:GLN:HG3	1:A:331:GLN:HE22	1.70	0.53
1:A:335:GLN:HE21	1:A:354:ILE:HG21	1.71	0.53
1:A:267:VAL:HG23	1:A:267:VAL:O	2.08	0.53
1:A:113:ARG:O	1:A:116:ALA:HB3	2.07	0.53
1:A:184:ASP:O	1:A:217:TRP:HA	2.08	0.53
1:A:42:ASP:OD1	1:A:44:THR:N	2.37	0.53
1:A:189:HIS:HA	1:A:222:ASP:O	2.08	0.53
1:A:350:PHE:HA	1:A:352:PHE:CE1	2.44	0.53
1:A:25:ARG:CZ	1:A:25:ARG:O	2.57	0.52
1:A:23:LEU:H	1:A:23:LEU:CD1	2.22	0.52
1:A:76:ILE:HB	1:A:79:PHE:CB	2.40	0.52
1:A:370:VAL:HG11	1:A:383:ALA:HA	1.90	0.52
1:A:375:GLU:CG	1:A:376:GLU:H	2.21	0.52
1:A:404:ILE:N	1:A:404:ILE:HD13	2.25	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ASN:C	1:A:165:ASN:OD1	2.47	0.52
1:A:223:PHE:O	1:A:254:SER:HA	2.09	0.52
1:A:121:LYS:HZ2	1:A:122:ASN:CB	2.23	0.52
1:A:350:PHE:C	1:A:352:PHE:N	2.62	0.52
1:A:145:SER:O	1:A:149:SER:HB3	2.10	0.52
1:A:202:LEU:O	1:A:206:GLN:HG3	2.09	0.52
1:A:373:LEU:HB3	1:A:379:VAL:HG22	1.92	0.52
1:A:160:TYR:O	1:A:168:LEU:HA	2.10	0.52
1:A:59:TYR:O	1:A:63:ASN:HB2	2.09	0.52
1:A:363:SER:OG	1:A:365:LEU:HG	2.09	0.51
1:A:205:TRP:HE3	1:A:205:TRP:HA	1.70	0.51
1:A:54:LYS:HA	1:A:57:GLU:HG3	1.92	0.51
1:A:121:LYS:NZ	1:A:122:ASN:CB	2.74	0.51
1:A:9:ILE:HG23	1:A:9:ILE:O	2.11	0.51
1:A:119:LEU:HG	1:A:125:VAL:HG21	1.92	0.51
1:A:67:THR:OG1	1:A:69:ASN:HB2	2.10	0.51
1:A:109:THR:HG22	1:A:140:TRP:HH2	1.72	0.51
1:A:397:MET:HA	1:A:400:LEU:HD23	1.91	0.51
1:A:162:ASP:O	1:A:163:ALA:HB3	2.10	0.51
1:A:94:LEU:HD23	1:A:94:LEU:O	2.11	0.51
1:A:121:LYS:C	1:A:123:THR:N	2.63	0.50
1:A:42:ASP:OD2	1:A:46:LYS:NZ	2.44	0.50
1:A:223:PHE:CE2	1:A:226:GLN:HB2	2.47	0.50
1:A:256:TYR:HB2	1:A:267:VAL:HG21	1.92	0.50
1:A:209:ALA:HB2	1:A:243:PHE:CE1	2.46	0.50
1:A:17:ILE:CG1	1:A:18:LEU:N	2.69	0.50
1:A:135:VAL:C	1:A:158:TYR:CE2	2.85	0.50
1:A:168:LEU:O	1:A:170:PHE:N	2.45	0.50
1:A:101:ARG:HG2	1:A:280:VAL:CG1	2.42	0.50
1:A:224:ALA:O	1:A:225:TYR:CB	2.60	0.50
1:A:29:ARG:HB3	1:A:30:PRO:HD2	1.92	0.49
1:A:17:ILE:C	1:A:19:GLY:H	2.09	0.49
1:A:404:ILE:N	1:A:404:ILE:CD1	2.75	0.49
1:A:24:PHE:CZ	1:A:33:ILE:CA	2.91	0.49
1:A:363:SER:O	1:A:365:LEU:N	2.45	0.49
1:A:353:ILE:HD12	1:A:353:ILE:O	2.12	0.49
1:A:90:LYS:HA	1:A:90:LYS:HZ3	1.78	0.49
1:A:29:ARG:CB	1:A:30:PRO:HD2	2.43	0.49
1:A:165:ASN:O	1:A:167:THR:N	2.46	0.49
1:A:99:ARG:NH2	1:A:274:ALA:O	2.45	0.49
1:A:180:ALA:O	1:A:181:GLN:CB	2.53	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:ARG:O	1:A:116:ALA:N	2.47	0.48
1:A:217:TRP:CD1	1:A:217:TRP:N	2.80	0.48
1:A:19:GLY:O	1:A:20:LEU:CB	2.56	0.48
1:A:278:GLU:OE1	1:A:282:ARG:NH2	2.47	0.48
1:A:220:LEU:CD1	1:A:251:ILE:HG12	2.44	0.48
1:A:44:THR:HG22	1:A:44:THR:O	2.14	0.47
1:A:135:VAL:O	1:A:136:SER:CB	2.60	0.47
1:A:256:TYR:HA	1:A:259:ASN:OD1	2.15	0.47
1:A:334:ARG:HB3	1:A:353:ILE:HD12	1.96	0.47
1:A:30:PRO:HG2	1:A:30:PRO:O	2.14	0.47
1:A:158:TYR:HD1	1:A:173:LEU:HD13	1.80	0.47
1:A:121:LYS:HE2	1:A:286:GLN:HB3	1.96	0.47
1:A:140:TRP:HE3	1:A:143:HIS:CD2	2.33	0.47
1:A:197:GLY:HA3	1:A:357:ASN:H	1.80	0.47
1:A:49:VAL:O	1:A:49:VAL:HG22	2.14	0.47
1:A:32:LYS:HB3	1:A:32:LYS:HE3	1.74	0.47
1:A:62:GLU:CG	1:A:63:ASN:HD22	2.28	0.47
1:A:119:LEU:HD12	1:A:119:LEU:HA	1.70	0.47
1:A:43:GLU:OE2	1:A:333:MET:CE	2.63	0.47
1:A:105:THR:CG2	1:A:107:GLY:HA2	2.45	0.47
1:A:140:TRP:CZ2	1:A:142:ASN:HB3	2.50	0.46
1:A:344:LYS:HD3	1:A:344:LYS:O	2.14	0.46
1:A:99:ARG:O	1:A:280:VAL:HG21	2.15	0.46
1:A:211:LEU:HD22	1:A:211:LEU:HA	1.66	0.46
1:A:106:PRO:HA	1:A:266:ARG:O	2.15	0.46
1:A:350:PHE:C	1:A:352:PHE:H	2.18	0.46
1:A:80:GLY:O	1:A:81:ARG:C	2.53	0.46
1:A:160:TYR:O	1:A:169:ASP:N	2.46	0.46
1:A:32:LYS:NZ	1:A:400:LEU:HD22	2.30	0.46
1:A:210:GLN:O	1:A:211:LEU:C	2.53	0.46
1:A:248:LYS:O	1:A:273:VAL:HG23	2.16	0.46
1:A:54:LYS:O	1:A:57:GLU:N	2.48	0.45
1:A:32:LYS:CE	1:A:400:LEU:HB2	2.41	0.45
1:A:71:LEU:HA	1:A:71:LEU:HD12	1.77	0.45
1:A:88:PHE:HA	1:A:241:ARG:HD2	1.98	0.45
1:A:352:PHE:O	1:A:356:GLN:NE2	2.50	0.45
1:A:121:LYS:C	1:A:121:LYS:CD	2.82	0.45
1:A:160:TYR:OH	1:A:198:ILE:O	2.30	0.45
1:A:177:LEU:HA	1:A:177:LEU:HD12	1.51	0.45
1:A:398:ALA:HB3	1:A:399:PRO:HD2	1.98	0.45
1:A:266:ARG:HH21	1:A:266:ARG:HD2	1.38	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:ILE:C	1:A:10:THR:OG1	2.55	0.45
1:A:352:PHE:O	1:A:356:GLN:HG3	2.17	0.45
1:A:225:TYR:HE1	3:A:410:PLP:O3	1.99	0.45
1:A:127:ARG:HH11	1:A:181:GLN:CD	2.21	0.44
1:A:338:VAL:HG21	1:A:354:ILE:HG23	1.99	0.44
1:A:248:LYS:HZ2	1:A:248:LYS:CB	2.02	0.44
1:A:9:ILE:HD13	1:A:10:THR:CA	2.47	0.44
1:A:353:ILE:HD12	1:A:353:ILE:C	2.38	0.44
1:A:15:ASP:OD2	1:A:17:ILE:HG22	2.18	0.44
1:A:185:VAL:HA	1:A:218:LEU:O	2.18	0.44
1:A:262:LEU:O	1:A:263:TYR:C	2.56	0.44
1:A:304:SER:O	1:A:305:VAL:C	2.55	0.44
1:A:118:PHE:O	1:A:121:LYS:NZ	2.49	0.44
1:A:25:ARG:HA	1:A:25:ARG:HD2	1.69	0.44
1:A:344:LYS:HA	1:A:344:LYS:HD3	1.57	0.44
1:A:152:LEU:HD12	1:A:152:LEU:HA	1.79	0.44
1:A:397:MET:HE3	1:A:400:LEU:CD2	2.48	0.44
1:A:322:GLU:O	1:A:325:ASP:HB2	2.18	0.44
1:A:106:PRO:HD2	1:A:295:TYR:CZ	2.53	0.44
1:A:31:GLY:C	1:A:33:ILE:H	2.21	0.44
1:A:20:LEU:HD13	1:A:382:VAL:HA	1.98	0.44
1:A:222:ASP:OD1	3:A:410:PLP:N1	2.51	0.44
1:A:328:GLN:HA	1:A:331:GLN:NE2	2.32	0.44
1:A:53:VAL:HG13	1:A:305:VAL:HG11	2.00	0.43
1:A:312:ASN:ND2	1:A:312:ASN:C	2.71	0.43
1:A:15:ASP:O	1:A:17:ILE:CG2	2.66	0.43
1:A:328:GLN:HG3	1:A:331:GLN:HE21	1.79	0.43
1:A:40:TYR:CZ	1:A:326:MET:HG2	2.52	0.43
1:A:32:LYS:CD	1:A:400:LEU:HB2	2.49	0.43
1:A:15:ASP:O	1:A:17:ILE:HG22	2.18	0.43
1:A:121:LYS:HZ2	1:A:122:ASN:HB3	1.84	0.43
1:A:123:THR:HG21	1:A:125:VAL:HG22	1.98	0.43
1:A:316:ARG:HH21	1:A:316:ARG:HD2	1.69	0.43
1:A:274:ALA:HB1	1:A:279:THR:HB	2.01	0.43
1:A:375:GLU:C	1:A:377:PHE:N	2.72	0.43
1:A:260:PHE:HB3	1:A:262:LEU:HD12	1.99	0.43
1:A:140:TRP:CE3	1:A:143:HIS:CD2	3.07	0.43
1:A:380:TYR:N	1:A:380:TYR:CD1	2.86	0.42
1:A:133:VAL:O	1:A:155:VAL:HA	2.19	0.42
1:A:393:THR:H	1:A:396:ASN:ND2	2.17	0.42
1:A:219:PRO:O	1:A:251:ILE:HG22	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:PHE:HE2	1:A:226:GLN:HB2	1.82	0.42
1:A:319:TRP:CZ2	1:A:323:LEU:HD22	2.55	0.42
1:A:205:TRP:CE3	1:A:205:TRP:CA	2.98	0.42
1:A:112:LEU:HA	1:A:112:LEU:HD23	1.58	0.42
1:A:127:ARG:HD2	1:A:134:TRP:NE1	2.35	0.42
1:A:156:ARG:HH22	1:A:179:GLU:CD	2.23	0.42
1:A:243:PHE:O	1:A:247:HIS:CD2	2.73	0.42
1:A:121:LYS:HZ3	1:A:122:ASN:HB2	1.84	0.42
1:A:375:GLU:O	1:A:377:PHE:N	2.52	0.42
1:A:23:LEU:O	1:A:27:ASP:N	2.39	0.42
1:A:212:SER:HA	1:A:217:TRP:CE3	2.55	0.42
1:A:24:PHE:C	1:A:26:ALA:H	2.22	0.41
1:A:44:THR:CB	1:A:46:LYS:NZ	2.77	0.41
1:A:373:LEU:O	1:A:378:GLY:N	2.53	0.41
1:A:87:LEU:HD22	1:A:240:LEU:HD11	2.01	0.41
1:A:315:LEU:HD12	1:A:315:LEU:HA	1.75	0.41
1:A:195:PRO:CB	1:A:362:PHE:HE1	2.17	0.41
1:A:310:LEU:HD12	1:A:316:ARG:CZ	2.50	0.41
1:A:136:SER:HB3	1:A:158:TYR:CZ	2.55	0.41
1:A:220:LEU:HA	1:A:251:ILE:O	2.21	0.41
1:A:220:LEU:HB2	1:A:251:ILE:CG2	2.51	0.41
1:A:194:ASN:HA	1:A:195:PRO:HA	1.90	0.41
1:A:40:TYR:OH	1:A:326:MET:HA	2.21	0.41
1:A:37:ILE:HG21	1:A:37:ILE:HD13	1.77	0.41
1:A:103:ALA:O	1:A:269:ALA:CB	2.67	0.41
1:A:220:LEU:HD13	1:A:251:ILE:HG12	2.03	0.41
1:A:372:ARG:NH1	1:A:375:GLU:OE2	2.53	0.41
1:A:366:THR:HG22	1:A:369:GLN:CD	2.41	0.41
1:A:108:GLY:HA3	3:A:410:PLP:O2P	2.20	0.41
1:A:399:PRO:O	1:A:402:GLU:HB3	2.20	0.41
1:A:325:ASP:O	1:A:326:MET:C	2.60	0.41
1:A:119:LEU:HB3	1:A:125:VAL:HG21	2.03	0.41
1:A:291:ILE:C	1:A:293:ALA:N	2.72	0.41
1:A:51:THR:O	1:A:55:LYS:HG3	2.21	0.41
1:A:76:ILE:O	1:A:79:PHE:HB3	2.21	0.40
1:A:101:ARG:HG2	1:A:280:VAL:HG13	2.03	0.40
1:A:174:ILE:HD13	1:A:174:ILE:HA	1.89	0.40
1:A:15:ASP:HA	1:A:16:PRO:HD3	1.69	0.40
1:A:32:LYS:HE2	1:A:400:LEU:CB	2.47	0.40
1:A:233:LEU:HD21	1:A:319:TRP:CZ3	2.55	0.40
1:A:270:CYS:SG	1:A:287:MET:CE	3.09	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:LEU:HD12	1:A:373:LEU:HA	1.86	0.40
1:A:324:THR:O	1:A:328:GLN:HB2	2.22	0.40
1:A:233:LEU:HD12	1:A:233:LEU:HA	1.69	0.40
1:A:370:VAL:O	1:A:374:ARG:HG3	2.22	0.40
1:A:218:LEU:HA	1:A:219:PRO:HD3	1.85	0.40
1:A:260:PHE:CZ	1:A:310:LEU:CD2	2.99	0.40
1:A:86:LEU:HA	1:A:86:LEU:HD23	1.73	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	394/396 (100%)	319 (81%)	44 (11%)	31 (8%)	1 2

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	ALA
1	A	13	PRO
1	A	17	ILE
1	A	29	ARG
1	A	33	ILE
1	A	50	LEU
1	A	90	LYS
1	A	136	SER
1	A	160	TYR
1	A	166	HIS
1	A	192	CYS
1	A	217	TRP
1	A	9	ILE
1	A	20	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	30	PRO
1	A	97	ASP
1	A	107	GLY
1	A	163	ALA
1	A	164	GLU
1	A	182	ALA
1	A	197	GLY
1	A	364	GLY
1	A	383	ALA
1	A	8	ASN
1	A	92	SER
1	A	263	TYR
1	A	266	ARG
1	A	180	ALA
1	A	27	ASP
1	A	375	GLU
1	A	80	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	320/320 (100%)	231 (72%)	89 (28%)	0 1

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	9	ILE
1	A	17	ILE
1	A	18	LEU
1	A	20	LEU
1	A	22	ASP
1	A	23	LEU
1	A	25	ARG
1	A	27	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	30	PRO
1	A	32	LYS
1	A	34	ASN
1	A	35	LEU
1	A	43	GLU
1	A	46	LYS
1	A	47	THR
1	A	61	LEU
1	A	62	GLU
1	A	71	LEU
1	A	86	LEU
1	A	97	ASP
1	A	98	LYS
1	A	99	ARG
1	A	101	ARG
1	A	105	THR
1	A	109	THR
1	A	113	ARG
1	A	119	LEU
1	A	121	LYS
1	A	125	VAL
1	A	126	LYS
1	A	127	ARG
1	A	136	SER
1	A	139	SER
1	A	149	SER
1	A	152	LEU
1	A	157	GLU
1	A	162	ASP
1	A	167	THR
1	A	173	LEU
1	A	177	LEU
1	A	179	GLU
1	A	185	VAL
1	A	188	PHE
1	A	196	THR
1	A	198	ILE
1	A	201	THR
1	A	205	TRP
1	A	208	LEU
1	A	210	GLN
1	A	211	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	218	LEU
1	A	220	LEU
1	A	223	PHE
1	A	234	GLU
1	A	235	GLU
1	A	240	LEU
1	A	243	PHE
1	A	248	LYS
1	A	252	VAL
1	A	255	SER
1	A	264	ASN
1	A	271	THR
1	A	273	VAL
1	A	277	SER
1	A	278	GLU
1	A	280	VAL
1	A	297	ASN
1	A	304	SER
1	A	312	ASN
1	A	320	GLU
1	A	327	ARG
1	A	329	ARG
1	A	335	GLN
1	A	339	ASN
1	A	343	GLU
1	A	344	LYS
1	A	348	ARG
1	A	351	SER
1	A	355	LYS
1	A	371	LEU
1	A	372	ARG
1	A	373	LEU
1	A	375	GLU
1	A	384	SER
1	A	386	PHE
1	A	396	ASN
1	A	402	GLU
1	A	404	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	104	GLN
1	A	122	ASN
1	A	166	HIS
1	A	181	GLN
1	A	206	GLN
1	A	247	HIS
1	A	264	ASN
1	A	312	ASN
1	A	331	GLN
1	A	335	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PLP	A	410	1	15,15,16	1.74	3 (20%)	21,22,23	2.80	10 (47%)
2	SO4	A	411	-	4,4,4	2.16	3 (75%)	6,6,6	1.42	1 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PLP	A	410	1	-	0/6/6/8	0/1/1/1
2	SO4	A	411	-	-	0/0/0/0	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	410	PLP	C5-C4	-3.72	1.36	1.40
3	A	410	PLP	C4A-C4	-3.36	1.44	1.51
3	A	410	PLP	O3-C3	-2.50	1.31	1.37
2	A	411	SO4	O2-S	2.26	1.54	1.47
2	A	411	SO4	O1-S	2.31	1.55	1.47
2	A	411	SO4	O4-S	2.50	1.56	1.47

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	410	PLP	C5-C6-N1	-3.12	118.44	123.86
3	A	410	PLP	O3P-P-O1P	-2.95	101.09	110.58
3	A	410	PLP	O2P-P-O4P	-2.74	98.68	106.56
3	A	410	PLP	C3-C2-N1	-2.25	117.50	120.61
3	A	410	PLP	C2A-C2-N1	2.02	122.43	117.95
3	A	410	PLP	C6-N1-C2	2.78	124.95	119.28
3	A	410	PLP	C4A-C4-C5	2.78	123.78	120.88
2	A	411	SO4	O4-S-O3	3.15	121.79	108.98
3	A	410	PLP	O4P-P-O1P	3.61	116.33	107.14
3	A	410	PLP	O2P-P-O1P	4.62	125.45	110.58
3	A	410	PLP	O4P-C5A-C5	8.18	122.52	108.99

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	410	PLP	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	396/396 (100%)	-0.89	0 100 100	12, 12, 12, 12	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	SO4	A	411	5/5	0.96	0.20	1.57	12,12,12,12	0
3	PLP	A	410	15/16	0.97	0.18	0.20	12,12,12,12	0

6.5 Other polymers

There are no such residues in this entry.